

## **Hydrogen Bonding Under High-Pressure**

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**M. Riad Manaa and Laurence E. Fried**

**Physical and Life Sciences Directorate  
Lawrence Livermore National Laboratory**

**P.O.Box 808, L-282, Livermore, CA, 94551**

**Email:manaa1@llnl.gov**

### **ABSTRACT**

Triamino-trinitro-benzene (TATB,  $C_6H_6N_6O_6$ ) exhibits unusually strong intramolecular hydrogen bonding as evidenced by the high rotational energy barrier of the nitro and amino groups. In the condensed phase, the competing intermolecular hydrogen bonding becomes pronounced at high-pressure in its graphitic-like crystal structure. In this talk, I will present the results of first-principal computational studies concerning the effect of isotropic high-pressure on the atomistic structure and the electronic properties of TATB up to 250 GPa. Along a specific crystal lattice direction, there exists a pressure regime where both the inter and intra-molecular hydrogen bonding become close, but still distinct. Comparison with formic acid, which undergoes polymerization at a much lower pressure regime, will be made. Further, possible mechanisms of phase transitions in the lower pressure regime of up to 50 GPa of TATB will be discussed, along with comparison with experimental high-pressure X-ray diffraction studies.

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